Zijie Wu

Education

- **Ph.D. in Chemical & Biomolecular Engineering**   08/2018 - 11/2023
  University of Delaware
  Thesis advisor: Prof. Arthi Jayaraman

- **B.Sc. in Chemical & Biomolecular Engineering** *with High Distinction*   08/2013 - 12/2017
  University of Illinois, Urbana-Champaign
  Minor degree in Computer Science

Professional Experience

- **Postdoctoral Research Fellow**   12/2023 -
  Data NanoAnalytics Group, Center for Nanophase Materials Science, Oak Ridge National Lab

- **Research Intern**   06/2023 - 08/2023
  Schrödinger, Inc.

Honors and Awards

- AIChE Excellence in Graduate Student Research Symposium, Area 08A – Finalist   2023
- American Physical Society (APS) DPOLY Padden Award – Finalist   2023
- James Scholar
  Dept. of Chemical Engineering, University of Illinois, Urbana-Champaign   2013 - 2017
- Chester W. Hanuum Chemical Engineering Fellowship
  Dept. of Chemical Engineering, University of Illinois, Urbana-Champaign   2017

Peer-reviewed Publications

(# denotes equal contributions)

- **Z. Wu**, A. M. Collins, A. Jayaraman, Understanding self-assembly and molecular packing in methylcellulose aqueous solutions using multiscale modeling and simulations, *submitted to Biomacromolecules*
- **Z. Wu**, J. W. Wu, Q. Michaudel, A. Jayaraman, Investigating Hydrogen Bond Induced Polysulfamide Self-assembly Aided by Molecular Simulations and Experiments, *Macromolecules* 56, 13, 5033-5049 (2023)
- **Z. Wu,** A. Jayaraman, Machine Learning Enhanced Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) for Analyzing Fibrillar Structures in Solutions, *Macromolecules* 55, 24, 11076-11091 (2022)
- Z. Ye, **Z. Wu**, A. Jayaraman, Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) on Vesicles Assembled from Amphiphilic Macromolecular Solutions, *JACS Au* 1, 11, 1925-1936 (2021)
- S. Lu#, **Z. Wu**#, A. Jayaraman, Molecular Modeling and Simulation of Polymer Nanocomposites with Nanorod Fillers, *J. Phys Chem B* 125, 9, 2435–2449 (2021)
- **Z. Wu**, D. Beltran-Villegas, A. Jayaraman, Development of a New Coarse-Grained Model to Simulate Assembly of Cellulose Chains Due to Hydrogen Bonding, *Journal of Chemical Theory and Computation* 16, 7, 4599–4614 (2020)

Conference Presentations

- **Z. Wu**, A. M. Collins, A. Jayaraman, Understanding Fibrillar Structure and Chain Packing in Methylcellulose Solutions Using Machine Learning, Genetic Algorithm and Multiscale Simulations (Talk), Excellence in Graduate Student Research Symposium, Area 08A, AIChE Annual Meeting (2023)
- **Z. Wu *(on behalf of A. Jayaraman)***, A. Jayaraman, C. Heil, Machine learning enhanced computational reverse-engineering analysis for scattering experiments (CREASE) of soft materials to establish structure-property relationships, American Physical Society (APS) Annual Meeting (2023)
- **Z. Wu**, A. Jayaraman, Machine Learning Enhanced Computational Reverse-Engineering Analysis of Scattering Experiments (CREASE) and Molecular Modeling for Analyzing Fibrillar Structures in Methylcellulose Solutions (Talk), Padden Award Symposium, American Physical Society (APS) Annual Meeting (2023)
- **Z. Wu**, A. Jayaraman, Computational and Experimental Study Linking Polysulfamide Chain Design to the Hydrogen Bonding Induced Chain Aggregation (Talk), Materials Research Society (MRS) Fall Meeting (2022)
- **Z. Wu**, A. Jayaraman, Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) on Biomacromolecular Assemblies (Talk), MRS Fall Meeting (2022)
- **Z. Wu**, A. Jayaraman, A New Computational Method (CREASE) to Analyze and Interpret Small Angle Scattering Profiles from Assembled Structure in Polymer Solutions (Talk), American Conference on Neutron Scattering (2022)
- **Z. Wu**, J. W. Wu, Q. Michaudel, A. Jayaraman, Computational Study Linking Polysulfamide Chain Design to the Hydrogen Bonding Induced Chain Aggregation (Talk), American Physical Society (APS) Annual Meeting (2022)
- **Z. Wu**, A. Jayaraman, Computational Reverse-Engineering Analysis for Scattering Experiments (CREASE) on Thermoresponsive Assembly of Methylcellulose in Aqueous Solutions (Poster), APS Annual Meeting (2022)
- **Z. Wu**, A. Jayaraman, Development of a Coarse-Grained Model to Simulate Assembly within Solutions of Cellulose and Cellulose Derivatives (Talk), Virtual MRS Spring Meeting (2021)
- **Z. Wu,** A. Jayaraman, A Coarse-Grained Model Capturing Hydrogen Bonding Effect in Cellulose and Its Derivatives (Talk), Virtual AIChE Annual Meeting (2020)
- **Z. Wu**, A. Jayaraman, Development of a New Coarse-Grained Model Capturing Hydrogen Bonding Effects in Polysaccharides (Talk), AIChE Annual Meeting (2019)

Other Academic Experience

- **Hackathon:** Data-based modeling of polymer blend formulations (2022)
  - *Part of the 2022 UD CBE course "CHEG 867-015: Computing and Data Science for Soft Materials Innovation and Design"*
  - *Developed models based on real, industrial datasets from DuPont to link polymer blend compositions to properties*

Professional Service

- **Seminar/Workshop:** A Tutorial for CREASE - a Computational Method for Analysis of Small Angle Scattering Results (virtual, co-hosted with NIST)
  - *Lead the workshop that introduces the CREASE method and its related open-source python package, CREASE-GA, to scattering scientists at NIST*
- **Mentoring:** Mentor of three first year graduate student in the Jayaraman group during their 1st year of PhD

Open-access Software Packages

- **CREASE-GA** (leader) – an open-source python framework to interpret small-angle scattering profile without relying on analytical model https://github.com/arthijayaraman-lab/crease_ga/
- **Molecular Simulation Design Framework** (Contributor, leader of the Univ. of Delaware team) – Python tools to facilitate the initialization, atom-typing, and screening of soft matter systems using molecular simulation https://mosdef.org

Teaching Experience

University of Delaware

- **Fall 2023, Fall 2022** Guest Lecturer – CHEG 867 Molecular Modeling and Simulation of Soft Materials
- **Fall 2020, Fall 2019** Teaching Assistant, Chemical Engineering Senior Lab – Distillation

University of Illinois, Urbana-Champaign

- **Spring 2017** Teaching Assistant, Principles of Chemical Engineering